

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.623

Global applicability domain: Inside

Local applicability domain index: 6.51e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

Image not found

NSC226971

Measured: -0.630

Predicted: -0.623

Image not found

Isopropyl beta-D-1-thiogalactopyranoside

Measured: -1.26

Predicted: -1.16